Project Quality Assurance Plan

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ASCEM

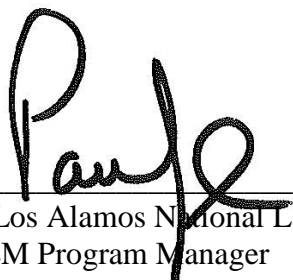## United States Department of Energy

E M Environmental Management

safety ❖ performance ❖ cleanup ❖ closure

Approval:

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2

Table of Contents

Tables

Figures

3

1.   SCOPE

1.1. Project Background

The Advanced Simulation Capability for Environmental Management (ASCEM) project (the "Project") brings together significant National Laboratory expertise in environmental and computational systems science to develop an advanced modeling capability for resolving contaminant release, transport, fate, and remediation issues across the Department of Energy (DOE) Environmental Management (EM) complex. The multidisciplinary, multi-institutional team will develop an open source modeling platform within a state-of-the-art high performance computing (HPC) framework to produce the next generation simulation software needed to address the prediction, risk reduction, and decision support challenges faced by DOE-EM sites. The Project will provide the next generation performance assessment capability and provide technical underpinnings for less complex models where they can be applied.

The Project will develop an integrated approach that bridges the technical and computational gaps that have often led to poor representation of complex systems, poor utilization of existing data, and suboptimal expenditure in the collection of new data. Conceptually accurate models and tools will be implemented to comprise a modeling platform with an HPC framework and several user application toolsets that together will allow full integration between data, simulations, and uncertainty quantification. ASCEM will be based on DOE-EM needs and will leverage significant advances both in scientific HPC (made through investments by the DOE Office of Science, the Nuclear Energy Advanced Modeling and Simulation (NEAMS) initiative, the Accelerated Strategic Computing Initiative (ASCI), and others) and in fundamental understanding of contaminant transport and fate (made through Office of Science Biological and Environmental Research investments).

The project includes three key technical thrust areas:

1. Platform and Key Toolsets
2. Multi-Process HPC Simulator
3. Site Applications.

Each thrust area is further organized into tasks, and activities supporting the tasks, all of which lead to deliverables.

The Platform and HPC framework will integrate and maximize new concepts, approaches and software, drive the migration of simulations to the most capable high-performance computers available, and encourage a standardization of approach that will best serve DOE-EM's long-term mission needs. The HPC software architecture will be "born parallel" to enable implementation

4

and extension on current and future HPC machines. The Site Applications thrust, in close collaboration with DOE site contractor and regulatory personnel, will lead the testing of the developed capabilities.

The Project is funded by the DOE EM-32 and is a collaborative effort between:
- Pacific Northwest National Laboratory (PNNL)
- Los Alamos National Laboratory (LANL)
- Lawrence Berkeley National Laboratory (LBNL)
- Oak Ridge National Laboratory (ORNL)
- Savannah River National Laboratory (SRNL)
- With technical support from:
  - Argonne National Laboratory (ANL)
  - Idaho National Laboratory (INL)
  - Lawrence Livermore National Laboratory (LLNL).

Additional discussion and information is contained in the ASCEM Implementation Plan[1].

1.2. Quality Assurance

This ASCEM Project Quality Assurance Plan (PrQAP) provides the upper tier Quality Assurance (QA)/Software Quality Assurance (SQA) requirements for the Project (i.e., the relationship between the governing documents and the Project).

Implementation Quality Assurance Plans (QAP) will be developed to meet the requirements contained in this PrQAP and will provide the implementation details for each of the requirements herein.

An ASCEM PrQAP Programmatic document will provide the administrative requirements for the ASCEM Project (e.g., assessments).

Responsibilities related to the PrQAP are defined in various ASCEM documents (e.g., implementation software quality assurance plans) and this plan. The individuals responsible for establishing and executing the PrQAP may delegate any or all of the work to others, **but shall retain responsibility thereof**.

The requirements contained in this PrQAP will satisfy the requirements of:

- DOE Order 414.1C

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1. FY2010 Initiative Implementation Plan: Advanced Simulation Capability for Environmental Management (ASCEM) (WBS 1.1.), March 18, 2010.

- 10 CFR 830 (when applicable) - The table below (in this Section) provides the relationship of the 10 criteria of the DOE documents and the 18 NQA-1-2004 (with the 2005 and 2007 addenda) Nuclear Quality Assurance criteria

- DOE-EM Quality Assurance Program; EM-QA-001

- ANSI/ASME NQA-1.

Table 1 below provides the relationship of the 10 criteria of the DOE documents and the 18 criteria of NQA-1-2004 (with the 2005 and 2007 addenda).

ASCEM program activities will evolve over time as processes are more fully understood and agreement on technical direction is determined. For this reason, Subpart 4.2 (Sp 4.2) of NQA-1 will be used to enhance the graded application of the requirements applicable to ASCEM. Figures 1, 2, and 3 provide a graphic of the gradation of requirements that will be used on ASCEM.

The structure of this PrQAP reflects the graded application of NQA-1, provided in Subpart 4.2 of NQA-1. Specifically, Subpart 4.2 recognizes the Basic, Applied, and Development Phases of software development. The high-level software requirements for the three Phases are identified in three Appendices attached to this PrQAP. Implementation SQA Plans will be developed to provide the implementation specifics for each of the Appendices (Phases). A description of each Phase follows:

- *Basic Phase –* Appendix A: The objective of the activities/efforts at this Phase is to gain a more complete knowledge or understanding of the fundamental aspects of phenomena and of observable facts (i.e., modeling capability for resolving contaminant release, transport, fate, and remediation issues across the EM complex).

- *Applied Phase –* Appendix B: The objective of activities/efforts at this Phase is to gain knowledge or understanding necessary for determining the means by which a recognized and specific need maybe met (i.e., modeling capability for resolving contaminant release, transport, fate, and remediation issues across the EM complex).

- *Development Phase –* Appendix C: (This is the phase at which software activities move from the graded approach recommended in Subpart 4.2, to a graded approach using NQA-1 for software.) The objective of activities/efforts at this Phase is the development, procurement, maintenance, and use of software for the ASCEM software activities. The Quality Assurance requirements are designed to fulfill the work practice requirements of NQA-1-2004 (including addenda 2005, and 2007), Subpart 2.7, and the software requirements of Part I (i.e., Requirement 3, paragraph 400 and 800, and Requirement 11, paragraph 400).

An ASCEM Programmatic Plan to support the PrQAP, which contains the requirements for Project support activities (e.g., auditing, training, document control), is approved and issued. The Programmatic Plan provides a graded approach (e.g., applicability of NQA-1 requirements to the Project) for the ASCEM Project. Implementation SQA Plans will provide additional grading

6

(e.g., when and to what degree processes are applicable for that phase).

With this PrQAP structure, users of the PrQAP can locate the area specific to their activity.

Table 1. *Relationships of 10 DOE QA Documents Mapped Against 18 Criteria of NQA-1-2004 (with the 2005 and 2007 addenda).*

NQA-1 Req. / DOE QA Criteria	1. Organization	2. QA Program	3. Design Control	4. Proc. Doc. Control	5. Instructions, Procedures, & Drawings	6. Document Control	7. Control Purchased Items & Services	8. Ident. & Control of Items	9. Control of Spec. Processes	10. Inspection	11. Test Control	12. Control of Measuring & Test Equip.	13. Handling, Storage, & Shipping	14. Inspect., Test & Operating Status	15. Control of Nonconformances	16. Corrective Action	17. QA Records	18 Audits
1. Program	X	X																
2. Training & Qualification		X																
3. Quality Improvement		X													X	X		
4. Documents & Records					X	X											X	
5. Work Processes					X			X	X			X	X	X				
6. Design			X															
7. Procurement				X			X											
8. Inspect. & Accept. Test								X		X	X	X						
9. Management Assess.		X																X
10. Independent Assess.	X	X								X	X				X	X		X

ASCEM Project activities are software oriented; there are no hardware-type activities (e.g., welding). As such, the requirements defined in this PrQAP are SQA requirements and other QA requirements that support those efforts (e.g., records, auditing). Project QA requirements are contained in several locations:

- ASCEM Project Quality Assurance Plan
    - Implementation Software Quality Assurance Plans (developed to meet requirements from PrQAP appendices)
- ASCEM Programmatic Plan (provides the requirements for Project support activities, such as document control and auditing).

The non-software requirements, or general requirements, applicable to the Project (regardless of the Phase) are described below:

1.2.1.   NQA-1, Requirement 3, Organization:

Project organization is defined in the ASCEM Implementation Plan[2].

1.2.2.   NQA-1, Requirement 3, Quality Assurance Program:

This PrQAP provides the appropriate QA requirements for the Project. The requirement basis for this Project is NQA-1-2004 (with the 2005 and 2007 addenda), graded for the Project's activities, which will meet the requirements of the DOE EM Quality Assurance Plan (EM-QAP-001). As discussed previously and shown in Table 1, this will also meet the requirements of DOE O 414.1C (and 10CFR830, as appropriate).

Subpart 4.2 of NQA-1, *Guidance on Graded Application of the Nuclear Quality Assurance (NQA) for Research and Development*, provides guidance on utilizing NQA-1 on research and development activities, as well as a methodology for grading NQA-1. Since the Project efforts evolve from research activities to the production of deliverable software, Subpart 4.2 was used to provide the structure for the PrQAP. The ASCEM Programmatic Plan contains a supplement (Supplement 1) that provides two matrices: a matrix on the breakdown of NQA-1-2004 (with the 2005 and 2007 addenda) to the ASCEM Project; and a matrix of Subpart 4.2 and the Project.

1.2.3.   NQA-1, Requirement 3, Training:

The requirements for this element of NQA-1 requirement are applicable to the Project's software activities. However, the formalization of training activities is not required until the activities are entering the *Development* phase. Training requirements are identified in the ASCEM implementation documents. The specific, formalized requirements will be defined in the Implementation SQA Plans, having been developed to meet the requirements defined in the appendices to this PrQAP.

1.2.4.   NQA-1, Requirement 3, Design Control:

This requirement of NQA-1 is applicable to the Project's software activities. General information is provided in this section, and the specific requirements are contained in the appendices to this PrQAP.

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2. FY2010 Initiative Implementation Plan: Advanced Simulation Capability for Environmental Management (ASCEM) (WBS 1.1.), March 18, 2010.

8

During the Basic Phase:
- Development defined
- Configuration Management
- Peer Review (testing).

During the Applied Phase:
> NQA-1
- Requirement 3, paragraph 800
- Requirement 11, software req. (e.g., 400).

During the Development Phase:
> NQA-1
- Req. 3 (800), Req. 11 (Software)
- Subpart 2.7
- Subpart 4.1.

> DOE O 414.1C
- Safety Software (full).

The transition of activities from one phase to another is defined in the ASCEM Implementation Plan[3].

1.2.5.   NQA-1, Requirement 3, Procurement Document Control:

Participating National Laboratories shall utilize their existing procurement and subcontract policies and processes. For procurements and subcontracts of items or services that effect quality, the procurements or subcontracts shall be routed through the ASCEM Project Manager and Lead Project Quality Engineer to assure a) conformity with project objectives, and b) that appropriate QA requirements and specifications are included and will be administered.

1.2.6.   NQA-1, Requirement 5, Instructions, Procedures, and Drawings:

Examples of instructions, procedures, and drawings (documents) on the ASCEM Project are:
- PrQAP
- Implementation Software Quality Assurance Plan

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3. FY2010 Initiative Implementation Plan: Advanced Simulation Capability for Environmental Management (ASCEM) (WBS 1.1.), March 18, 2010.

9

- User Guide
- Tech Procedures/Test Plans – except for Basic doc.

Other documents, such as procedures and instructions, may be developed based on implementation requirements contained in documents like the Implementation Software Quality Assurance Plan.

1.2.7.   NQA-1, Requirement 6, Document Control:

Examples of documents that will be controlled on the ASCEM Project are:
- PrQAP
- Implementation Software Quality Assurance Plan
- User Guide
- Tech Procedures/Test Plans – except for Basic doc.

Other documents, such as procedures and instructions, will require control based on implementation requirements contained in documents like the Implementation Software Quality Assurance Plan.

1.2.8.   NQA-1, Requirement 7, Control of Purchased Items and Services:

Participating National Laboratories shall utilize their procurement and subcontract policies and processes. For procurements and subcontracts of items or services that effect quality, the procurements or subcontracts shall be routed through Project Manager and Lead Project Quality Engineer to assure a) conformity with project objectives, and b) that appropriate quality assurance requirements and specifications are included and will be administered.

1.2.9.   NQA-1, Requirement 8, Identification and Control of Items:

For this project, which is software oriented, these requirements are not applicable.

1.2.10.   NQA-1, Requirement 9, Control of Special Processes:

For this project, which is software oriented, these requirements are not applicable.

1.2.11.   NQA-1, Requirement 10, Inspection:

For this project, the application of this requirement pertains to the performance of surveillances (see ASCEM Programmatic Plan, Supplement 1).

10

1.2.12. NQA-1, Requirement 11, Test Control:

This requirement of NQA-1 is applicable to the software activities of the project. The specific requirements are contained in the appendices to this PrQAP.

1.2.13. NQA-1, Requirement 12, Control of Measuring and Test Equipment:

For this project, which is software oriented, these requirements are not applicable.

1.2.14. NQA-1, Requirement 13, Handling, Storage, and Shipping:

For this project, which is software oriented, these requirements are not applicable.

1.2.15. NQA-1, Requirement 14, Inspection, Test, and Operating Status:

For this project, which is software oriented, these requirements are not applicable.

1.2.16. NQA-1, Requirement 15, Control of Nonconforming Items:

This requirement of NQA-1 is applicable to the Project software activities (e.g., deficiency reports). The specific requirements are contained in the appendices to this PrQAP.

1.2.17. NQA-1, Requirement 16, Corrective Action:

This requirement of NQA-1 is applicable to the Project software activities. The specific requirements will be defined in implementation documentation such as the Implementation Software Quality Assurance Plan and the ASCEM Programmatic Plan.

1.2.18. NQA-1, Requirement 17, Quality Assurance Records:

This requirement of NQA-1 is applicable to the project. The ASCEM Project Manager shall assure that Project records are controlled in accordance with the PNNL records practices defined in the PNNL Lab-level web-based system.

1.2.19. NQA-1, Requirement 18, Audits:

The ASCEM Programmatic Plan provides specifics on this requirement for the project.

11

NOTE: All Phases can be executed concurrently.

Basic Phase
(Evolutionary Model. All new features and functionality are vetted in Basic Phase.)

Define Basic Phase requirements

A

Create and document design

Implement

Test/Review

Model is correct?
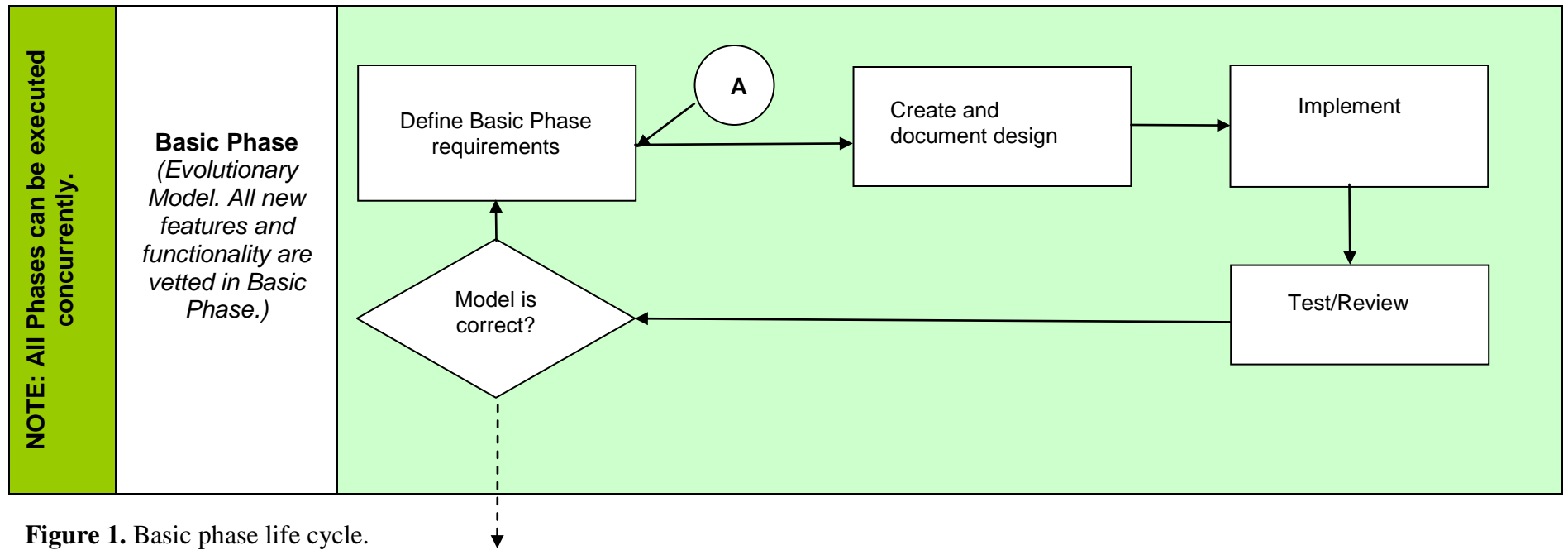
Figure 1. Basic phase life cycle.
This life cycle is independent of other Phases.
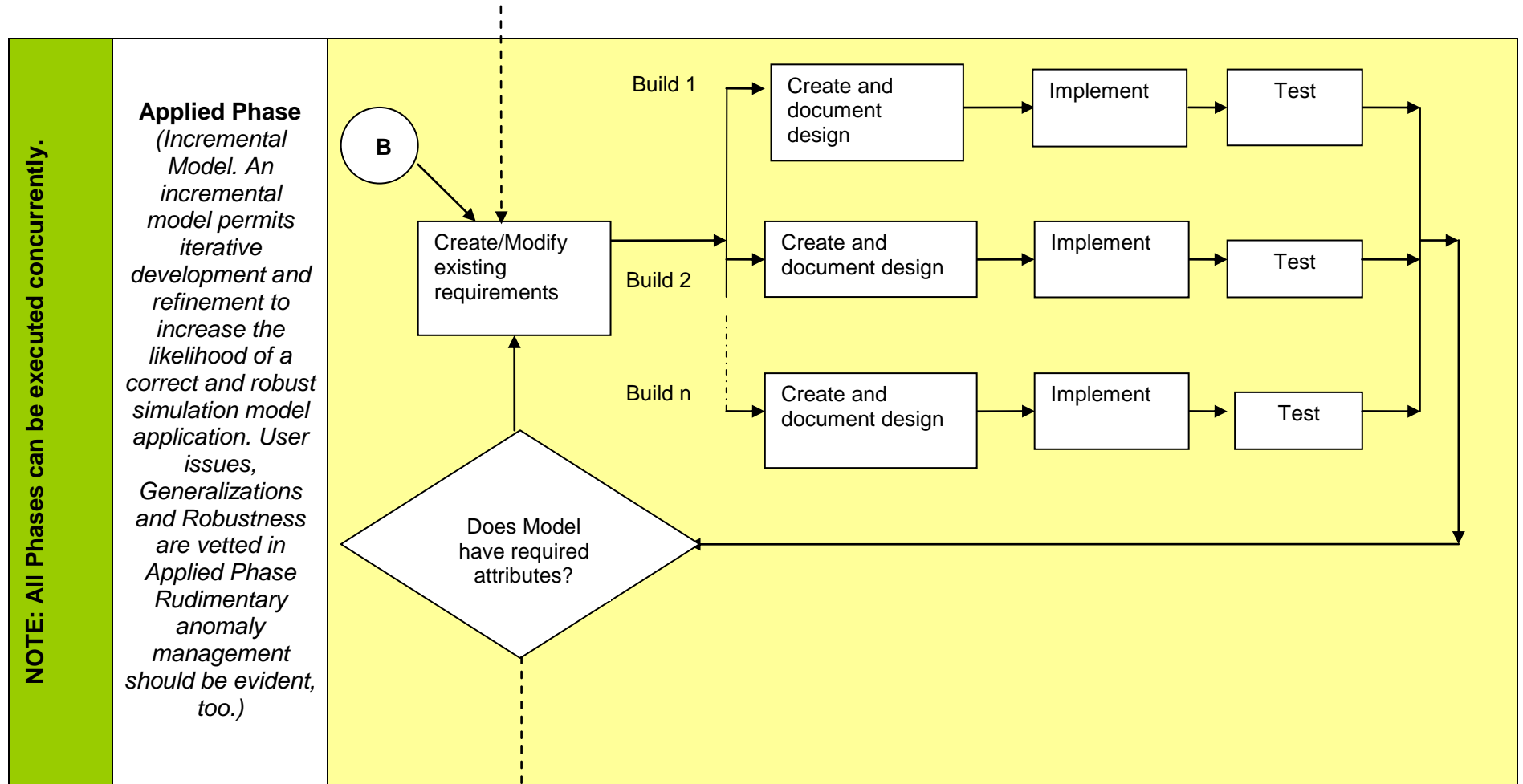
Figure 2. Applied phase life cycle.
This life cycle is independent of other Phases.

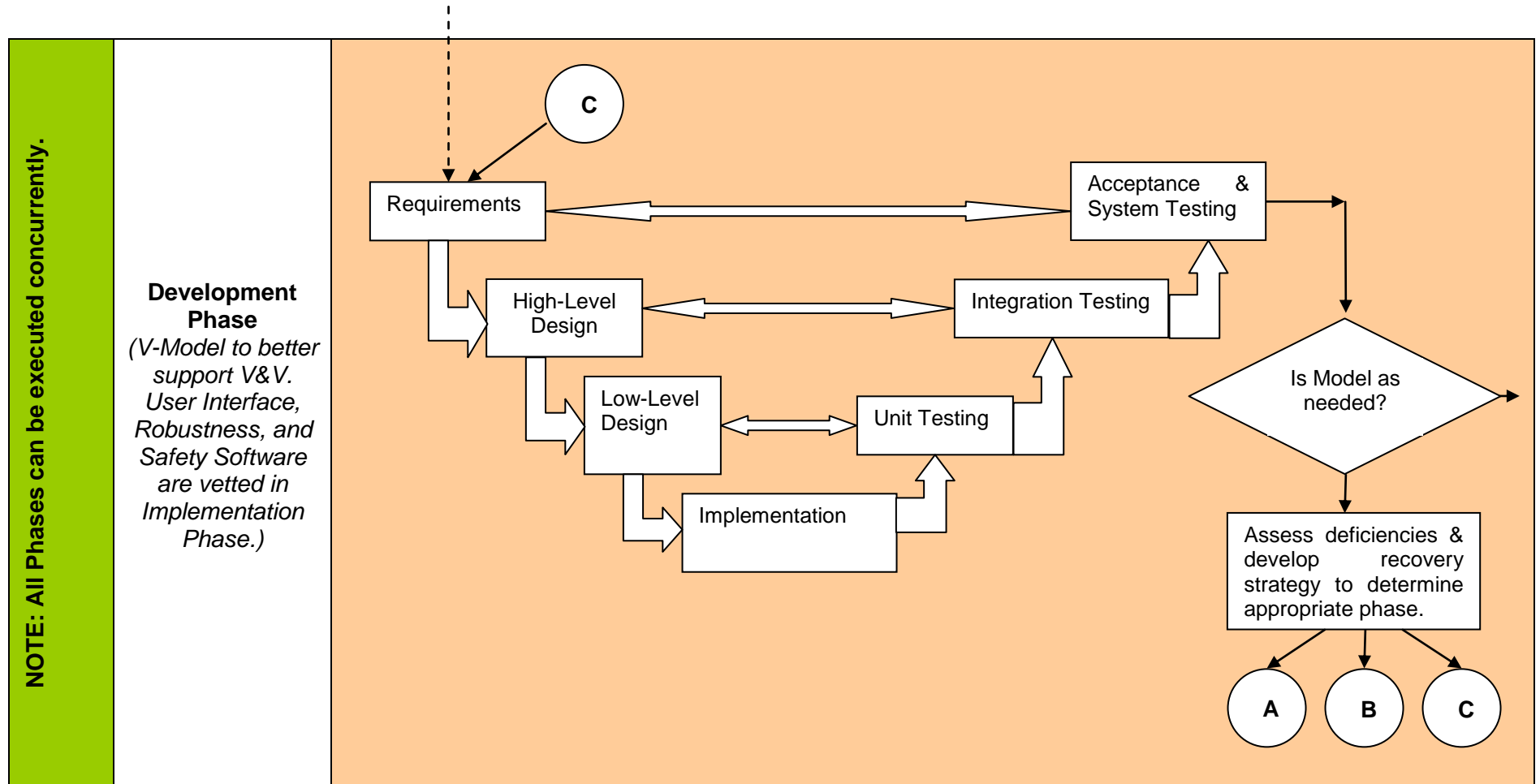**Figure 3.** Development phase life cycle.
This life cycle is independent of other Phases.

APPENDIX A – ACRONYMS AND ABBREVIATIONS

ASCEM	Advanced Simulation Capacity for Environmental Management
DOE	Department of Energy
EM	Environmental Management
HPC	High Performance Computing
NQA	Nuclear Quality Assurance
PrQAP	Project Quality Assurance Plan
QA	Quality Assurance
QAP	Quality Assurance Plan
RBGA	Risk-Based Graded Approach
SQA	Software Quality Assurance

APPENDIX B – QA REQUIREMENTS, BASIC PHASE

INTRODUCTION

This Appendix contains the quality assurance (QA) requirements for the development, procurement, maintenance, and use of software, for the software activities in the *Basic Phase* of the ASCEM Project (the "Project"). The Quality Assurance requirements contained in this Appendix have been developed using NQA-1-2004 (addenda 2005 and 2007) Subpart 4.2, *Guidance on Graded Application of Quality Assurance (QA) for Nuclear-Related Research and Development*, for software.

At the Basic Phase of the ASCEM Project, the objective of the activities/efforts is to gain more complete knowledge or understanding of the fundamental aspects of phenomena and of observable facts (i.e., modeling capability for resolving contaminant release, transport, fate, and remediation issues across the EM complex).

The management controls (implementation specifics) for the QA requirements contained in this Appendix are detailed in a separate Software Quality Assurance Plan – Basic Phase (B-SQAP). The B-SQAP provides the detailed implementation for the requirements in this Appendix, and will be supported by other implementation documents (e.g., the Configuration Management Plan).

The requirements in this Appendix **consider** the requirements for safety software, where the Project has deemed them to be appropriate based on a graded approach (i.e., considering potential future use). It is important to recognize that the Safety Software elements at this phase are very elemental (DOE Order 414.1C [DOE O 414.1C] and DOE Guide 414.1-4 [DOE G 414.1-4] provide requirements and guidance regarding Safety Software) because safety software requirements are not applicable at this phase of the Project (Safety Software requirements have been determined to be applicable during the Development Phase of the ASCEM Project).

Section 1 – Basic Phase Software Requirements

1.1 Define the development

- Documentation of requirements and algorithms is sufficient for this Research and Development phase of software development:
  - Requirements (i.e., what are the program's objectives?)
  - High-level design
  - Associated documentation (i.e., design and requirements documents).

1.2 Configuration Management
The thrust lead shall ensure that the basic phase software development will:

- Maintain a master repository of the software using a modern version control system.
- Locate the master repository on a server that resides in a room with controlled access, and for which backups are maintained.
- Implement a tagging scheme for identifying specific versions of the software, and ensure version tagging may be output by the code.
- Maintain a list of developers with access to the source code.

The software developer shall use established best-practices for basic phase (i.e., R&D) code development, including:

- Develop all relevant code under version control, contributing their advances regularly to the master repository (e.g., commit/push).
- Document objectives and progress on development activities through project management and version control tools (e.g., ticket system, commit messages).
- Implement and document tests (unit/verification) as an integral part of the development process, problem reporting, and corrective action (e.g., use of automated tracking tools such Trac and MercurialHG).

1.3   Internal Peer Review (testing)

The developer shall ensure that the software product (i.e., computer program, user manual) receives at least one Peer Review prior to moving the software product to an Integrated Demonstration. (An integrated demonstration will consist of the necessary software testing, verification, and validation required to demonstrate the coupling between 2 or more software components or subsystems to achieve one or more of the ASCEM goals.) The developer shall ensure the technical peer review of the software product includes:

- The technical approach used is adequately described
- The methodology is sound and replicable
- The data and analyses used are well supported and appropriate for the conclusions drawn
- There are no obvious errors of fact or logic
- There is appropriate acknowledgement of the work of others
- The software product is at the appropriate professional level for the intended use, and it will enhance the ASCEM objectives.

Peer reviewers for technical documents will be chosen based on knowledge and experience of the potential reviewers relevant to the subject matter.

External stakeholder testing activities will not occur until release of User Release Version 1.0 of code to the stakeholders, which is currently scheduled for December, 2011.

APPENDIX C – QA REQUIREMENTS, APPLIED PHASE

INTRODUCTION

This appendix contains the quality assurance requirements for the development, procurement, maintenance, and use of software, for the software activities in the *Applied Phase* of the ASCEM Project. The Quality Assurance (QA) requirements contained in this Appendix have been developed using NQA-1-2004 (addenda 2005 and 2007) Subpart 4.2, *Guidance on Graded Application of Quality Assurance (QA) for Nuclear-Related Research and Development*, for software.

At the Applied Phase of the ASCEM Project, the objective of the activities/efforts is to gain knowledge or understanding necessary for determining the means by which a recognized and specific need maybe met (i.e., modeling capability for resolving contaminant release, transport, fate, and remediation issues across the EM complex).

The management controls (implementation specifics) for the QA requirements contained in this Appendix are detailed in a separate Software Quality Assurance Plan – Applied Phase (A-SQAP). The A-SQAP provides the detailed implementation for the requirements in this Appendix, and will be supported by other implementation documents (e.g., Configuration Management Plan).

The requirements in this Appendix provide a graded approach to the requirements for safety software (DOE Order 414.1C [DOE O 414.1C] and DOE Guide 414.1-4 [DOE G 414.1-4] provide requirements and guidance regarding Safety Software) because safety software requirements are not fully applicable at this phase of the Project (Safety Software requirements have been determined to be fully applicable during the Development Phase of the ASCEM Project).

The requirements for this phase shall be developed in a later revision to the ASCEM PrQAP, but prior to any software efforts requiring *Application Phase* requirements.

APPENDIX D – QA REQUIREMENTS, DEVELOPMENT PHASE

INTRODUCTION

This appendix contains the quality assurance (QA) requirements for the development, procurement, maintenance, and use of software, for the software activities in the *Development Phase* of the ASCEM Project (the "Project"). The QA requirements contained in this Appendix are designed to fulfill the work practice requirements of NQA-1-2004 (including addenda 2005, and 2007), Subpart 2.7, and the software requirements of Part I (i.e., Requirement 3, paragraph 400 and 800, and Requirement 11, paragraph 400).

At the Development Phase of the ASCEM Project, the application of the understanding gained from the earlier phases (Basic, Applied) will be applied to meet the ultimate ASCEM Project objectives (i.e., modeling capability for resolving contaminant release, transport, fate, and remediation issues across the EM complex).

The management controls (implementation specifics) for the QA requirements contained in this Appendix are detailed in a separate Software Quality Assurance Plan – Development Phase (D-SOAP). The D-SQAP provides the detailed implementation for the requirements in this Appendix, and will be supported by other implementation documents (e.g., Configuration Management Plan).

In 2005, the Department of Energy (DOE) issued DOE Order 414.1C (DOE O 414.1C) and DOE Guide 414.1-4 (DOE G 414.1-4), which provided requirements and guidance regarding Safety Software. The full Safety Software elements of DOE O 414.1C and DOE G 414.1-2 have been integrated into the requirements of this Development Phase.

The requirements for this phase shall be developed in a later revision to the ASCEM PrQAP, but prior to any software efforts requiring *Development Phase* requirements.